

Carbonic acid, but-3-en-1-yl octyl ester

Inchi:	InChI=1S/C13H24O3/c1-3-5-7-8-9-10-12-16-13(14)15-11-6-4-2/h4H,2-3,5-12H2,1H3
InchiKey:	VLBCFEVGRUTYNX-UHFFFAOYSA-N
Formula:	C13H24O3
SMILES:	C=CCCOC(=O)OCCCCCCCC
Mol. weight [g/mol]:	228.33

Physical Properties

Property code	Value	Unit	Source
gf	-192.50	kJ/mol	Joback Method
hf	-563.24	kJ/mol	Joback Method
hfus	32.12	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	4.076		Crippen Method
mvol	203.040	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	1533.00		NIST Webbook
rinpol	1533.00		NIST Webbook
tb	592.23	K	Joback Method
tc	763.38	K	Joback Method
tf	328.90	K	Joback Method
vc	0.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.30	J/molxK	592.23	Joback Method
cpg	537.88	J/molxK	620.75	Joback Method
cpg	552.83	J/molxK	649.28	Joback Method
cpg	567.16	J/molxK	677.80	Joback Method
cpg	580.87	J/molxK	706.33	Joback Method
cpg	593.97	J/molxK	734.85	Joback Method
cpg	606.47	J/molxK	763.38	Joback Method
dvisc	0.0019778	Paxs	328.90	Joback Method

dvisc	0.0009807	Paxs	372.79	Joback Method
dvisc	0.0005637	Paxs	416.68	Joback Method
dvisc	0.0003601	Paxs	460.56	Joback Method
dvisc	0.0002487	Paxs	504.45	Joback Method
dvisc	0.0001822	Paxs	548.34	Joback Method
dvisc	0.0001398	Paxs	592.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383229&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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